

REFERENCE POTENTIAL APPROACH TO THE QUANTUM-MECHANICAL INVERSE PROBLEM: I. CALCULATION OF PHASE SHIFT AND JOST FUNCTION

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ABSTRACT. Elegant and mathematically rigorous methods of the quantum inverse theory are difficult to put into practice because there is always some lack of needful input information. In this situation, one may try to construct a reference potential, whose spectral characteristics would be in a reasonable agreement with the available data of the system's properties. Since the reference potential is fixed, it is always possible to calculate all its spectral characteristics, including phase shift for scattering states and Jost function, the main key to solve the inverse problem. Thereafter, one can calculate a Bargmann potential whose Jost function differs from the initial one only by a rational factor. This way it is possible, at least in principle, to construct a more reliable potential for the system. The model system investigated in this paper is diatomic xenon molecule in ground electronic state. Its reference potential is built up of several smoothly joined Morse type components, which enables to solve the related energy eigenvalue problem exactly. Moreover, the phase shift can also be calculated in part analytically, and the Jost function can be ascertained very accurately in the whole range of positive energies. Full energy dependence of the phase shift has been determined and its excellent agreement with the Levinson theorem demonstrated. In addition, asymptotically exact analytic formulas for the phase shift and the Jost function, independent of each other, are obtained and their physical background elucidated.

1. INTRODUCTION

Strict mathematical criteria for the unique solution of the inverse problem for the one-dimensional Schrödinger equation have been formulated more than 50 years ago. The history of this prestigious research area goes back to the dawn of quantum mechanics [1], and the decisive breakthrough has been achieved thanks to the important contributions by Borg [2, 3], Levinson [4, 5], Bargmann [6, 7], Gel'fand and Levitan [8], Jost and Kohn [9, 10], Marchenko [11, 12], Krein [13, 14], and others (see, e.g., [15] for a thorough overview). As a result of fruitful brainstorming which culminated in early fifties it has been established that the quantum mechanical inverse problem can be solved if one manages to fix the so-called spectral function [11]. In the case of confining one-dimensional quantum systems it means that the interaction potential can be uniquely determined if and only if the following complete set of information is available:

- Full energy spectrum of the bound states E_n ($n = 0, 1, \dots, N$).
- Full energy dependence (from 0 to ∞) of the phase shift $\delta(E)$ for the scattering states $E > 0$.

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- n additional real parameters C_n ($n = 0, 1, \dots, N$) related to relevant bound states that uniquely fix their normalization.

In principle, all these data can be obtained experimentally, but unfortunately, this is almost unachievable in practice. The real situation is even more hopeless, because in addition to the deficit of input information one inevitably faces very serious computational-technical problems. Thus, in spite of the whole mathematical beauty of the theory, one comes to a regrettable conclusion that rigorous solution of the quantum-mechanical inverse problem is a tremendously difficult task. For this reason most methods of deducing potentials from the available experimental data are based on some simplifying preconditions, therefore being inaccurate from the rigorous quantum mechanical point of view. Nevertheless, such methods may prove quite useful. For example, semiclassical approaches introduced many years ago by Rydberg [17, 18], Klein [19], Rees [20] and Dunham [21, 22] are still very popular in spectroscopy of diatomic molecules, and these concepts are constantly improved and developed [23, 24].

Is it possible to apply rigorous methods of the inverse quantum theory for practical purposes? In view of the principle difficulties mentioned above, one has to be cautious in answering this question. In this paper we restrict ourselves to simple one-dimensional quantum systems, and the analysis proceeds from an idea that for any system of this kind one can build up a reasonable reference potential based on the available experimental data. As the reference potential is known, it is always possible to calculate all its discrete energy eigenvalues E_n , their norming constants C_n , and the phase shifts $\delta(E)$ for the scattering states. Therefore, in this artificial way one gets the full set of input information needed to uniquely solve the quantum mechanical inverse problem. Of course, the described approach is tautological: there is no need to regain a potential which is already known by definition. Nevertheless, such an approach is not meaningless, as it gives good zeroth approximations to the important spectral characteristics, such as *Jost function* and *spectral density* (the terms to be specified below). One can interpret the reference potential as only an initial guess to the real potential. Although the calculated quantities E_n , C_n and $\delta(E)$ do not exactly match the actual values for the real system, they are still expected to be quite close to them. For a given reference potential one can calculate its Bargmann potential whose Jost function differs from the initial one only by a rational factor [15]. By a suitable choice of this factor one can take a more adequate account of the experimental data. For example, one can replace the calculated discrete energy eigenvalues E_n related to the reference potential with their actually observed values. Consequently, at least in some sense the new potential would be more realistic than the initial reference potential. There is also another motivation for the described "inverse" approach to the inverse problem. Namely, through direct practical experience one can essentially increase his knowledge of how to overcome serious computational-technical difficulties when applying rigorous methods of the inverse quantum theory.

The one-dimensional inverse theory can be applied to diatomic molecules, since a two-particle problem can be always reduced to a one-particle problem in a spherically symmetric field. On this basis, we are going to examine the inverse problem for diatomic xenon molecule in its ground electronic state. Several reports of the research are planned. Methods of solution of the integral equations that enable to uniquely ascertain the potential are discussed and illustrated in the next paper of

this series [16], while in this paper the emphasis is put on explaining the details of the basic concepts related to the reference potential approach. In Section 2 we briefly describe how the reference potential for the model system has been constructed, and how its discrete energy eigenvalues have been calculated. In Section 3 we describe the details of calculating the phase shift for the scattering states, and demonstrate full agreement with Levinson theorem [4]. Section 4 aims to explain the important role of the Jost function in the quantum inverse theory. In particular, a detailed analysis of the asymptotic behavior of the Jost function is given. Finally, a brief conclusion is given in Section 5.

2. EXACTLY SOLVABLE REFERENCE POTENTIAL FOR Xe_2

In Fig. 1 one can see the reference potential constructed for the Xe_2 molecule. The same curve is depicted in both graphs, but very different energy scales are used. Throughout this paper only the rotationless case is analyzed, i.e., the rotational quantum number $J = 0$. According to the starting idea of the approach the only criterion for the choice of the reference potential is its agreement with the available experimental data. Therefore, we will not pay too much attention to various mathematical nuances and simply assume that the reference potential should be smooth and integrable in the whole physical domain. In addition, we try to construct a reference potential whose analytic form is as simple as possible. A good choice for this purpose, as explained in detail elsewhere [25, 26], is a multi-component potential composed of smoothly joined Morse-type pieces

$$(1) \quad V(r) = V_k + D_k [\exp(-\alpha_k(r - r_k)) - 1]^2, \quad r \in (0, \infty),$$

where V_k , D_k , α_k and r_k are some constants (not definitely positive), and the subscript k corresponds to different components smoothly joined at some suitably chosen boundary points X_{k+1} . The reference potential shown in Fig. 1 consists of only three components ($k = 0, 1, 2$), the most internal of them ($k = 0$) being a so-called pseudo-Morse potential. It means that the tiny potential well corresponding to this component (if taken separately) is just of the limit depth to entirely lose the discrete energy spectrum. Consequently, $D_0 = \hbar^2 \alpha_0^2 / (8m)$ (m being the reduced mass of the pair of atoms), so that only three independent parameters remain for this component. The central component ($k = 1$) is an ordinary Morse potential, while the most external one ($k = 2$) is a "reversed" Morse potential with the parameter D_2 being negative. By introducing a "reversed" component one artificially creates a small potential hump in the long-distance range. This might seem unphysical and unjustified, but the point is that the height of this artificial hump approaches zero as the parameter r_2 approaches infinity. Therefore, taking a sufficiently large r_2 , the hump becomes almost insignificant, while the analytic treatment remains simple and flexible. All parameters of the reference potential can be easily determined, if one requires continuity of the potential and its first derivative at the boundary points X_1 and X_2 (also shown in Fig. 1). These parameters as well as the calculated discrete energy eigenvalues E_n ($n = 0, 1, \dots, 23$) are given in Table 1.

The essence of the described construction is that the energy eigenvalue problem for the reference potential can be easily solved by solely analytic means to any desired accuracy [25]. Moreover, as we demonstrate in the next Section, the major

part of the energy dependence of the phase shift can also be ascertained analytically, which is a great advantage compared with applying numerical methods.

Most spectroscopic applications are related to the distance region shown in the lower graph of Fig. 1. For the inverse quantum theory, however, it is important to accurately reproduce the potential near the zero point $r = 0$, which is almost meaningless for spectroscopic applications. In this context one cannot ignore the fact that according to Eq. (1) the reference potential is finite at $r = 0$ (see the upper graph of Fig. 1). Actually it means that the potential "jumps" to infinity at zero point, and this might also seem unphysical and unjustified. However, one has to bear in mind that the behavior of the real potential near $r = 0$ is unknown and remains unknown. It does not matter so much how we describe the potential in this region, in so far as spectroscopic applications are of our main interest. As we see in the next section, description in terms of a pseudo-Morse potential is mathematically simple and elegant, and this, too, can be taken as a motivation for the approach to be used.

3. PHASE SHIFT AND LEVINSON THEOREM

Next we are going to calculate the phase shift $\delta(E)$ for the full range of scattering states $E \in (0, \infty)$. To this end, one can use a long-known method first introduced by Morse and Allis [27] (let us remind that only the rotationless case $J = 0$ is examined here). It is based on solution of the following equation:

$$(2) \quad \delta'(r, k) = -\frac{\sqrt{2m}V(r)}{\hbar k} \sin^2[kr + \delta(r, k)], \quad \delta(0, k) = 0,$$

where $k = \frac{\sqrt{2mE}}{\hbar}$. The phase shift is then determined as $\delta(k) = \lim_{r \rightarrow \infty} \delta(r, k)$. The described method is universal but rather time-consuming, because for any energy from 0 to ∞ one has to perform an integration from 0 to ∞ . Fortunately, at this point we can take advantage of the special analytic form of the reference potential. As mentioned, the region $r \in (0, X_1)$ is approximated by a pseudo-Morse potential. It means that one immediately gets two linearly independent analytic solutions of the corresponding Schrödinger equation [25, 26]

$$(3) \quad \begin{aligned} \Psi_0^{(1)}(r) &= \exp(-y_0/2) y_0^{i\mu_0} \Psi(i\mu_0, 2i\mu_0 + 1; y_0) \\ \Psi_0^{(2)}(r) &= \exp(y_0/2) (-y_0)^{i\mu_0} \Psi(i\mu_0, 2i\mu_0 + 1; -y_0), \quad r \in (0, X_1), \end{aligned}$$

where $\mu_0 = 1/2\sqrt{(E - V_0)/D_0 - 1} > 0$, $y_0 \equiv \exp[-\alpha_0(r - r_0)]$, and $\Psi(i\mu_0, 2i\mu_0 + 1; y_0)$ is a particular solution of the confluent hypergeometric equation introduced by Tricomi (see [28] for details). If $\mu_0^2 \ll y_0$, this function can be evaluated from the asymptotic series

$$(4) \quad \Psi(i\mu_0, 2i\mu_0 + 1; y_0) = y_0^{-i\mu_0} \sum_{n=0}^N \frac{(i\mu_0)_n (-i\mu_0)_n}{n! (-y_0)^n},$$

where $(a)_n \equiv \Gamma(a + n)/\Gamma(a) = a(a + 1)(a + 2) \dots (a + n - 1)$ is the Pochhammer symbol, and N must not be too large. Thus

$$(5) \quad \Psi_0^{(1)}(r) = \exp(-y_0/2) \left[1 - \frac{\mu_0^2}{1!y_0} + \frac{\mu_0^2(\mu_0^2 + 1^2)}{2!y_0^2} - \frac{\mu_0^2(\mu_0^2 + 1^2)(\mu_0^2 + 2^2)}{3!y_0^3} + \dots \right],$$

and analogously

$$(6) \quad \Psi_0^{(2)}(r) = \exp(y_0/2) \left[1 + \frac{\mu_0^2}{1!y_0} + \frac{\mu_0^2(\mu_0^2 + 1^2)}{2!y_0^2} + \frac{\mu_0^2(\mu_0^2 + 1^2)(\mu_0^2 + 2^2)}{3!y_0^3} + \dots \right].$$

The phase shift is related to *regular solutions* of the Schrödinger equation, which means that the physically correct linear combination of $\Psi_0^{(1)}(r)$ and $\Psi_0^{(2)}(r)$ should vanish as $r \rightarrow 0$, i.e.,

$$\Psi_0(r) = N_1 \Psi_0^{(1)}(r) + N_2 \Psi_0^{(2)}(r),$$

where

$$(7) \quad \frac{N_2}{N_1} = -\exp[-y_0(0)] \cdot \frac{1 - \frac{\mu_0^2}{1!y_0(0)} + \frac{\mu_0^2(\mu_0^2 + 1^2)}{2!y_0^2(0)} - \dots}{1 + \frac{\mu_0^2}{1!y_0(0)} + \frac{\mu_0^2(\mu_0^2 + 1^2)}{2!y_0^2(0)} + \dots}.$$

From Eq. (7) one can see that the particular solution $\Psi_0^{(2)}(r)$ practically does not contribute to the regular solution at distances sufficiently far from zero point, but still deep inside the classically forbidden region. Indeed, in this case

$$(8) \quad \frac{N_2 \Psi_0^{(2)}(r)}{N_1 \Psi_0^{(1)}(r)} = -\exp[y_0(r) - y_0(0)] \times \frac{1 - \frac{\mu_0^2}{1!y_0(0)} + \frac{\mu_0^2(\mu_0^2 + 1^2)}{2!y_0^2(0)} - \dots}{1 + \frac{\mu_0^2}{1!y_0(0)} + \frac{\mu_0^2(\mu_0^2 + 1^2)}{2!y_0^2(0)} + \dots} \times$$

$$\times \frac{1 + \frac{\mu_0^2}{1!y_0(r)} + \frac{\mu_0^2(\mu_0^2 + 1^2)}{2!y_0^2(r)} + \dots}{1 - \frac{\mu_0^2}{1!y_0(r)} + \frac{\mu_0^2(\mu_0^2 + 1^2)}{2!y_0^2(r)} - \dots} = -\exp[y_0(r) - y_0(0)] \times$$

$$\times \frac{1 + \frac{\mu_0^2}{1!y_0(0)} [\exp(\alpha_0 r) - 1] + \dots}{1 - \frac{\mu_0^2}{1!y_0(0)} [\exp(\alpha_0 r) - 1] + \dots} \approx -\exp\{-\exp(\alpha_0 r_0) [1 - \exp(-\alpha_0 r)]\}$$

is an extremely small quantity.

There is still a lot more profit to gain from the pseudo-Morse approximation to calculate the phase shift. As we just proved, the physically correct solution (apart from normalization) in a wide energy range (practically up to $E \approx V(0)$) reduces to the particular solution $\Psi_0^{(1)}(r)$. Using some well-known relations from the theory of confluent hypergeometric functions [28, 25] this solution can be rewritten

$$(9) \quad \Psi_0^{(1)}(r) = \exp(-y_0/2) y_0^{i\mu_0} \Psi(i\mu_0, 2i\mu_0 + 1; y_0) =$$

$$\exp(-y_0/2) \left[\frac{\Gamma(-2i\mu_0)}{\Gamma(-i\mu_0)} y_0^{i\mu_0} \Phi(i\mu_0, 2i\mu_0 + 1; y_0) + \frac{\Gamma(2i\mu_0)}{\Gamma(i\mu_0)} y_0^{-i\mu_0} \Phi(-i\mu_0, -2i\mu_0 + 1; y_0) \right],$$

where the symbols $\Phi(a, c; x) = 1 + \frac{a}{c} \frac{x}{1!} + \frac{a(a+1)}{c(c+1)} \frac{x^2}{2!} + \dots$ denote the well-known confluent hypergeometric functions.

As is seen, Eq. (9) represents a sum of two complex conjugates. Therefore,

$$\Psi_0^{(1)}(r) \sim A_0(y_0) \cos[B_0(y_0) - \varphi_0 - \alpha_0 \mu_0 r],$$

where the functions A_0 and B_0 can be determined from a series [25]:

$$(10) \quad A_0(y_0)e^{iB_0(y_0)} = 1 - \frac{y_0/4}{i\mu_0 + 1/2} + \frac{(y_0/4)^2}{(i\mu_0 + 1/2)1!} \left(1 - \frac{y_0/4}{i\mu_0 + 3/2}\right) + \\ + \frac{(y_0/4)^4}{(i\mu_0 + 1/2)(i\mu_0 + 3/2)2!} \left(1 - \frac{y_0/4}{i\mu_0 + 5/2}\right) + \dots$$

A good point is that the phase parameter (which, of course, is not the actual phase shift) $\varphi_0 \equiv \alpha_0\mu_0 r_0 - \arg \left[\frac{\Gamma(2i\mu_0)}{\Gamma(i\mu_0)} \right]$ can be calculated exactly. Indeed, using a Legendre formula for doubling a gamma function's argument [28]

$$\Gamma(2z) = \frac{2^{2z-1}}{\sqrt{\pi}} \Gamma(z) \Gamma(z + 1/2),$$

and another useful formula [29]

$$(11) \quad \arg \Gamma(i\mu_0 + 1/2) = \mu_0 \left(\frac{1}{2} \ln(1 + 4\mu_0^2) - 1 - \ln 2 \right) - \frac{1}{2} \int_0^\infty \left(\coth t - \frac{1}{t} \right) e^{-t} \sin(2\mu_0 t) \frac{dt}{t},$$

one gets the following result:

$$(12) \quad \varphi_0 = \mu_0 \left(\alpha_0 r_0 + 1 - \ln 2 - \frac{1}{2} \ln(1 + 4\mu_0^2) \right) + \frac{1}{2} \int_0^\infty \left(\coth t - \frac{1}{t} \right) e^{-t} \sin(2\mu_0 t) \frac{dt}{t},$$

where the integral can be conveniently evaluated [25]

$$(13) \quad I \equiv \int_0^\infty \left(\coth t - \frac{1}{t} \right) e^{-t} \sin(2\mu_0 t) \frac{dt}{t} = \int_0^T e^{-t} \sin(\pi \frac{t}{T}) f(t) dt, \quad T = \frac{\pi}{2\mu_0}, \\ f(t) = \frac{\coth t - \frac{1}{t}}{t} - e^{-T} \frac{\coth(t+T) - \frac{1}{t+T}}{t+T} + e^{-2T} \frac{\coth(t+2T) - \frac{1}{t+2T}}{t+2T} - \dots$$

Another equivalent formula for this quantity reads [26]

$$(14) \quad I = \sum_{n=1}^\infty I_n, \quad I_n = \frac{(-1)^{n-1} 2^{2n} B_n}{(2n)(2n-1)(1+4\mu_0^2)^{2n-1}} \sum_{k=0}^{n-1} (-1)^k \binom{2n-1}{2k+1} (2\mu_0)^{2k+1}.$$

Here B_n denotes the n -th order Bernoulli number.

Correct linear combinations of solutions of the Schrödinger equations for analytically different pieces of the reference potential are uniquely fixed by the continuity requirements of the wave function and its first derivative at the boundary points X_1 and X_2 . Since the parameter φ_0 can be calculated exactly, the phase shift can also be ascertained with the help of solely analytic means in the energy range $0 < E \lesssim V(0)$. At high energies ($E \gtrsim V(0)$), however, the analytic approach gradually fails, since the particular solution $\Psi_0^{(2)}(r)$ in Eq. (3) cannot be ignored any more. To determine the phase shift in this region one has to solve Eq. (2). Fortunately, there is no need to perform integration over the whole physical domain

$r \in (0, \infty)$, because the solution in the long-distance range $r \geq X_2$ already has the "right" analytic form [25]

$$(15) \quad \Psi_2(r) = 2A_2(y_2) \cos [B_2(y_2) + \varphi_2 - kr] = 2A_2(y_2) \sin [\delta(r, k) + kr],$$

from which the phase shift can be easily obtained. Here $y_2(r) \equiv 2a_2 \exp [-\alpha_2(r - r_2)]$, $a_2 \equiv \sqrt{2mD_2}/(\hbar\alpha_2)$, $\delta(r, k)$ is the solution of Eq. (2), and the complex function $A_2(y_2) \exp [iB_2(y_2)] \equiv \exp (-iy_2/2) \Phi [i(k/\alpha_2 - a_2) + 1/2, 2ik/\alpha_2 + 1; iy_2]$. Since $A_2(y_2) \rightarrow 0$ and $B_2(y_2) \rightarrow 1$ as $r \rightarrow 0$, the phase shift

$$(16) \quad \delta(k) = \delta(X_2, k) + B_2[y_2(X_2)],$$

i.e., one only needs to integrate Eq. (2) until the boundary point X_2 .

Now, let us recall an important relation known as Levinson theorem [4]

$$(17) \quad \delta(0) - \delta(\infty) = n\pi,$$

which correlates the energy dependence of the phase shift with the number of bound states. As can be seen in Fig. 2, a really good agreement with the Levinson theorem can be obtained, but only if the phase shift is calculated up to very high energies (note that the energy scale in Fig. 2 is logarithmic, and it involves 20 orders of magnitude!). Moreover, the phase shift has to be calculated with sufficiently high precision throughout the whole energy range, otherwise there is no chance to accurately ascertain other important spectral characteristics, such as Jost function. Unfortunately, the higher the energy goes, the more complicated and time-consuming the numerical integration of Eq. (2) becomes. How could we bridge over this troublesome technical difficulty? In such situation, one may recall some general principles, and this is indeed helpful to complete calculations of the phase shift.

Let us express the phase shift as formal result of integration of Eq. (2):

$$(18) \quad \begin{aligned} \delta(k) = \lim_{r \rightarrow \infty} \delta(r, k) = & -\frac{1}{2Ck} \int_0^\infty V(r) \{1 - \cos [2kr + 2\delta(r, k)]\} dr = -\frac{\int_0^\infty V(r) dr}{2Ck} + \\ & + \frac{1}{2Ck} \int_0^\infty \cos(2kr) \{V(r) \cos [2\delta(r, k)]\} dr - \frac{1}{2Ck} \int_0^\infty \sin(2kr) \{V(r) \sin [2\delta(r, k)]\} dr. \end{aligned}$$

Here a special denotation has been introduced (and will be used henceforward) for the constant $C \equiv \frac{\hbar^2}{2m}$ that often appears in formulas. Now, let us call for help from the famous Riemann-Lebesgue theorem (see, e.g., [30]): if a function $F(r)$ is integrable in an interval $r \in (a, b)$, then

$$(19) \quad \int_a^b \cos(\lambda r) F(r) dr \rightarrow 0, \quad \int_a^b \sin(\lambda r) F(r) dr \rightarrow 0 \text{ as } \lambda \rightarrow \infty.$$

From this one immediately concludes that the last two integrals in Eq. (18) will vanish as $k \rightarrow \infty$. However, we can integrate by parts and apply the Riemann-Lebesgue theorem to the resulting integrals. This procedure can be repeated as many times as needed, and as a result, one comes to a rather general asymptotic

formula for the phase shift (it can easily be proved that only odd powers of k appear in this series)

$$(20) \quad \delta(k) = \frac{a_1}{k} + \frac{a_3}{k^3} + \frac{a_5}{k^5} + \dots, \quad k \rightarrow \infty,$$

where

$$(21) \quad a_1 = -\frac{\int_0^\infty V(r)dr}{2Ck}, \quad a_3 = -\frac{1}{8C^2} \left\{ \int_0^\infty [V(r)]^2 dr + CV'(0) \right\},$$

$$a_5 = -\frac{1}{32C^3} \left\{ \int_0^\infty [V(r)]^3 dr + C \int_0^\infty [V'(r)]^2 dr + 4CV(0)V'(0) - C^2V'''(0) \right\}.$$

Thus one can easily calculate the coefficients a_1 , a_3 , a_5 , etc., and this is just what is needed to ascertain the whole energy dependence of the phase shift. Fig. 3 demonstrates how well Eq. (20) fits with the results of direct numerical integration of the phase equation.

One cannot so easily find any direct illustrations to the Levinson theorem from the literature (at least the author of this paper has not found them), and Fig. 2, which is an illustration of this kind, could therefore be of more general interest than merely an attachment to a particular model potential. The curve shown in this figure has been calculated with at least 8 significant digits, and it is in full agreement with all relevant general physical considerations. This concerns not only the Levinson theorem and the asymptotic behavior at large energies, but also the low energy part of the energy dependence (see the left-side inset of Fig. 2), exactly corresponding to the well-known formula

$$(22) \quad \delta(k) = n\pi - \arctan(kR_0), \quad k \rightarrow 0$$

(R_0 being scattering length), which can be found in most handbooks on quantum mechanics.

4. JOST FUNCTION AND INVERSE PROBLEM

Having calculated the phase shift, we have come to a situation from which an ideal inverse problem study would start. In other words, we are now provided with the full set of information needed to uniquely solve the inverse problem. In our case this would mean that we simply regain the reference potential from which we started. This, of course, is not our main goal. As explained in Section 1, we are interested in getting realistic zeroth approximations to the important spectral functions which then could be used to improve the initial model potential. The latter step, however, is planned as a subject for a forthcoming publication. In this paper we only try to make sure that the described scheme is reliable, and to this end the next step is to accurately calculate the Jost function, the main spectral characteristic, which contains the most part of information needed to solve the inverse problem. A thorough overview of all useful properties of the Jost function is given in Ref. [15]. For the treatment here, the most important point is that the Jost function creates a simple link between *physical* and regular solutions of the scattering states. The physical solution ($J = 0$) reads (cf. with Eq. (15))

$$(23) \quad \Psi(r, k) \approx \exp i\delta(k) \sin[kr + \delta(k)], \quad r \rightarrow \infty,$$

while the regular solution $\varphi(r, k)$ is defined by a condition

$$(24) \quad \lim_{r \rightarrow 0} \frac{\varphi(r, k)}{r} = 1.$$

It can be shown that these two solutions of the Schrödinger equation are proportional

$$(25) \quad \Psi(r, k) = \frac{k}{F(k)} \varphi(r, k),$$

where

$$(26) \quad F(k) = |F(k)| \exp[-i\delta(k)]$$

is the Jost function we are talking about. For further treatment we have to calculate the modulus of this function [15]

$$(27) \quad |F(E)| = \prod_{n=0}^N (1 - E_n/E) \exp \left[-\frac{1}{\pi} P \int_0^{\infty} \frac{\delta(E') dE'}{E' - E} \right], \quad E \in (0, \infty).$$

Here E_n are the discrete energy eigenvalues and the symbol P points at the principal value of the integral. As the phase shift and the bound states are known, the calculations are relatively trivial, but they have to be carried out very accurately. Next we can fix the spectral density

$$(28) \quad \frac{d\rho(E)}{dE} = \begin{cases} \pi^{-1} \sqrt{E} |F(E)|^{-2}, & E \geq 0, \\ \sum_n C_n \delta(E - E_n), & E < 0. \end{cases}$$

Here C_n are the norming constants for the relevant bound states. Note that these quantities are related to regular solutions, wherefore their ascertainment is not so easy task as one might think.

Now we have come close to the real solution schemes of the inverse problem. For example, the Gelfand-Levitan method [8] is based on the integral equation

$$(29) \quad K(r, r') + G(r, r') + \int_0^r K(r, s) G(s, r') ds = 0,$$

whose kernel reads

$$(30) \quad G(r, r') = \int_{-\infty}^{\infty} \frac{\sin(kr) \cdot \sin(kr')}{k^2} d\sigma,$$

and the quantity $d\sigma \equiv d\rho(E) - \frac{d\rho_0(E)}{dE} dE$. Here $\frac{d\rho_0(E)}{dE}$ is free particle's spectral density (related to the potential $V(r) \equiv 0$), and therefore,

$$(31) \quad d\sigma = \begin{cases} d\rho(E) - d\left(\frac{2E^{3/2}}{3\pi}\right), & E \geq 0 \\ d\rho(E), & E < 0. \end{cases}$$

Eq. (30) can be rewritten [15]

$$(32) \quad G(r, r') = \frac{2}{\pi} \int_0^{\infty} \sin(kr) \cdot \sin(kr') g(k) dk + \sum_n \frac{C_n}{4\gamma_n^2} \sinh(\gamma_n r) \sinh(\gamma_n r'),$$

where $\gamma_n^2 = -\frac{2mE_n}{\hbar^2}$ and the function

$$(33) \quad g(k) \equiv \frac{1}{|F(k)|^2} - 1.$$

If one is able to solve Eq. (29), the potential can be determined from the relation

$$(34) \quad V(r) = 2C \frac{d}{dr} K(r, r).$$

Eqs. (29) to (34) explicitly demonstrate great importance of the Jost function in the inverse quantum theory. The energy dependence of the Jost function's modulus is shown in Fig. 4. One can see that at small energies this quantity achieves extremely large values. Near the "critical" energy $E = V(0)$ the curve rapidly turns from nearly vertical to nearly horizontal, and at still higher energies it slowly approaches the limit value $|F(k)| \rightarrow 1$, "breaking free" from the potential field (note that for a free particle, $F(k) = 1$ independent of energy).

The kernel of the Gelfand-Levitan equation is essentially determined by the function $g(k)$ given by Eq. (33), which means that this function has to be ascertained very accurately, in order to solve Eq. (29) and calculate the potential according to Eq. (34). As can be seen in Fig. 5, $g(k)$ noticeably differs from unity only at $k \gtrsim k_0 \equiv \sqrt{V(0)/C}$, and $g(k) \rightarrow 0$ as $k \rightarrow \infty$. Naturally, as shown in the inset, there is no break of derivative in the "critical" region. Since the asymptotic behavior of the function $g(k)$ essentially determines the shape of the potential near the zero point $r = 0$ (see the end of this section), it makes sense to analyze this behavior in more details. We have already ascertained the asymptotic expression for the phase shift (see Eq. (20)), and this can be used to immediately get the asymptotic formulas for both the Jost function's modulus and the function $g(k)$. For example, taking

$$(35) \quad \ln |F(k)| = \frac{a_2}{k^2} + \frac{a_4}{k^4} + \frac{a_6}{k^6} + \dots, \quad k \rightarrow \infty$$

(this time only even powers of k appear in the series, as can be easily proved), the coefficients read

$$(36) \quad \begin{aligned} a_2 &= -\frac{2}{\pi} \left(a_1 k_a - \frac{a_3}{k_a} - \frac{a_5}{3k_a^3} - \dots \right) + \frac{1}{C} \left[\frac{1}{\pi} \int_0^{E_a} \delta(E') dE' - \sum_n E_n \right], \\ a_4 &= -\frac{2}{\pi} \left(\frac{a_1 k_a^3}{3} + a_3 k_a - \frac{a_5}{k_a} - \dots \right) + \frac{1}{C^2} \left[\frac{1}{\pi} \int_0^{E_a} \delta(E') E' dE' - \frac{1}{2} \sum_n (E_n)^2 \right], \\ a_6 &= -\frac{2}{\pi} \left(\frac{a_1 k_a^5}{5} + \frac{a_3 k_a^3}{3} + a_5 k_a - \dots \right) + \frac{1}{C^3} \left[\frac{1}{\pi} \int_0^{E_a} \delta(E') (E')^2 dE' - \frac{1}{3} \sum_n (E_n)^3 \right], \end{aligned}$$

where $E_a = Ck_a^2$ is an arbitrary energy value in the range where the asymptotic approximation Eq. (20) can be used.

Eq. (36) may look nice but it is a bit inconvenient in practice. Fortunately, a straightforward approach exists, which enables to ascertain the coefficients in Eq. (35) more accurately and much more easily without any direct reference to the phase

shift. The approach in question is based on the following integral representation for the Jost function [15]:

$$(37) \quad F(k) = 1 + \frac{1}{C} \int_0^\infty e^{ikr} V(r) \varphi(k, r) dr,$$

where the regular solution $\varphi(k, r)$ can be calculated with the help of a well-known iteration method. Namely, taking $\varphi^{(0)}(k, r) = \frac{\sin kr}{k}$, and

$$(38) \quad \varphi^{(n)}(k, r) = \frac{1}{C} \int_0^r \frac{\sin k(r-r')}{k} V(r') \varphi^{(n-1)}(k, r') dr', \quad n = 1, 2, \dots,$$

the desired solution reads

$$(39) \quad \varphi(k, r) = \sum_{n=0}^{\infty} \varphi^{(n)}(k, r).$$

In Eq. (38) one can use integration by parts to calculate step-by-step the terms $\varphi^{(1)}(k, r)$, $\varphi^{(2)}(k, r)$, $\varphi^{(3)}(k, r)$, ..., and their contributions to the Jost function. Let us see, how to ascertain the correct asymptotic formula for the function $g(k) = \frac{1}{|F(k)|^2} - 1$ as $k \rightarrow \infty$, which would include the terms until $\sim 1/k^4$. Within this approximation

(40)

$$\begin{aligned} \varphi^{(1)}(k, r) &= -\frac{\cos kr}{2Ck^2} W(r) + \frac{\sin kr}{4Ck^3} [V(0) + V(r)] + \frac{\cos kr}{8Ck^4} [V'(r) - V'(0)], \quad W(r) \equiv \int_0^r V(r') dr', \\ \varphi^{(2)}(k, r) &= -\frac{\sin kr \cdot [W(r)]^2}{8C^2k^2} - \frac{\cos kr}{8C^2k^4} [V(0)W(r) + V(r)W(r) + U(r)], \quad U(r) \equiv \int_0^r [V(r')]^2 dr', \\ \varphi^{(3)}(k, r) &= \frac{\cos kr \cdot [W(r)]^3}{48C^3k^4} \end{aligned}$$

(all higher order terms can be ignored). Thereafter, using integration by parts in Eq. (37), one comes to the following formulas for the real and imaginary parts of the Jost function:

(41)

$$\begin{aligned} \operatorname{Re} F(k) &= 1 + \frac{V(0)}{4Ck^2} - \frac{W^2}{8C^2k^2} - \frac{V''(0)}{16Ck^4} + \frac{1}{32C^2k^4} \left\{ 5[V(0)]^2 - 2V'(0)W \right\} - \\ &\quad - \frac{1}{32C^3k^4} [V(0)W^2 + 2UW] + \frac{W^4}{384C^4k^4}, \end{aligned}$$

$$(42) \quad \operatorname{Im} F(k) = \frac{W}{2Ck} + \frac{V'(0)}{8Ck^3} + \frac{1}{8C^2k^3} [V(0)W + U] - \frac{W^3}{48C^3k^3},$$

where $W \equiv \int_0^\infty V(r') dr'$ and $U \equiv \int_0^\infty [V(r')]^2 dr'$. Quite surprisingly, when calculating $|F(k)|^2 = [\operatorname{Re} F(k)]^2 + [\operatorname{Im} F(k)]^2$, all troublesome terms will cancel out, resulting

in nice expressions for both quantities of interest:

$$(43) \quad |F(k)|^2 = 1 + \frac{V(0)}{2Ck^2} + \frac{3[V(0)]^2}{8C^2k^4} - \frac{V''(0)}{8Ck^4},$$

$$(44) \quad g(E) = \frac{V(0)}{2E} + \frac{[V(0)]^2 - CV''(0)}{8E^2}.$$

Comparing Eqs. (35) and (44), one finds that the coefficients

$$(45) \quad a_2 = \frac{V(0)}{4C}, \quad a_4 = \frac{2[V(0)]^2 - CV''(0)}{16C^2}$$

do not depend on the phase shift, but are directly related to the potential and its second derivative at the zero point, both these quantities being finite according to the starting idea of the approach. Thus we have described all properties of the Jost function in the frame of the proposed approach, and are now prepared to start calculation of the potential itself.

5. CONCLUSION

In this paper we proposed as if an "inversed" approach to the quantum mechanical inverse problem. Starting from a known reference potential, one can calculate the important spectral characteristics of the system, the phase shift and the Jost function, which are almost unattainable in a real experiment. On one hand, the reference potential has to be realistic enough to be used as a zeroth approximation to the real potential. Only in this case there is a chance to construct a Bargmann potential that would be even more realistic, for example, whose discrete energy levels would exactly fit with the actually observed ones. On the other hand, we suggest to choose a reference potential that would be exactly solvable, in the sense that its energy eigenvalue problem can be solved to any desired accuracy with the help of solely analytic means. To this end, as demonstrated in Sections 2 and 3, a multi-component potential composed of smoothly joined Morse-type pieces is especially suitable. In particular, we would like to highlight the usefulness of the pseudo-Morse approximation for the small distances (and high energies) region of the potential. In this paper we only used a single pseudo-Morse component, which stretches until the zero point $r = 0$. As demonstrated elsewhere [25, 26], adding more pseudo-Morse components does not bring along any serious problems, so one can include just as many components of this type as he considers reasonable.

The special analytic form of the reference potential enables to ascertain the phase shift analytically up to the energies $E \lesssim V(0)$ (note that an arbitrarily large value for $V(0)$ can be taken, if one introduces a sufficient number of pseudo-Morse components). As the asymptotic behavior of the phase shift can be determined from general physical considerations, it is possible to directly demonstrate full agreement with the famous Levinson theorem [4], as well as to ascertain the full energy dependence of the Jost function. Provided with this important input information, one can attack the real computational-technical problem, trying to solve the main integral equation in the frame of the Gelfand-Levitan [8], Marchenko [12] or Krein [14] method. This will be the subject of the next paper in this series [16].

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FIGURE CAPTIONS

- Fig. 1. Three-component model potential for the system (Xe_2 in ground electronic state) investigated. Note that the same potential curve is depicted in both graphs (the lower one starts where the upper one ends), but essentially different energy scales are used for them. All components have the well-known analytic form of the Morse potential, but the ordinary Morse approximation is used only in the central range $r \in [X_1, X_2]$ (see the explanations in Section 2). The parameters of the components as well as the calculated discrete energy levels (24 in total) are given in Table 1.
- Fig. 2. Direct demonstration of the Levinson theorem ($\delta(0) - \delta(\infty) = n\pi$) for the model system studied. As needed, $\delta(0) = 24\pi$, since the system has 24 bound states. At $E = 3.146294$ meV, the phase shift passes a zero, and then remains negative, very slowly approaching the limit ($\delta(\infty) = 0$) as $E \rightarrow \infty$. The left side-inset shows the nearly linear energy dependence as $E \rightarrow 0$, in full agreement with Eq. (22). In the right-side inset one can see that the phase curve has an inflection point near $E = V(0)$.
- Fig. 3. A demonstration of the excellent agreement between the numerically calculated phase shifts and the general asymptotic formula, Eq. (20), as $E \rightarrow \infty$.
- Fig. 4. Demonstration of the results of calculating the Jost function (in fact, its modulus) for the reference potential. Again, as in the case of Fig. 1, different parts of the same curve are shown in the graphs and their insets, but rather different scales are used (note that in some cases the scale is logarithmic). The information gathered into the upper graph would be useful, if one's aim is to construct another potential whose Jost function only slightly differs from the initial one. The lower graph demonstrates how abruptly the curve turns from practically vertical to nearly horizontal in the vicinity of the "critical" energy value $E = V(0)$, while this dramatic change is absolutely invisible in the scale used for the ordinate axis in the upper graph. The asymptotic formula Eq. (35) is used to calculate the Jost function for $k \geq k_a = 75000 \text{ \AA}$ (which corresponds to about $1.8 \cdot 10^5$ eV) with coefficients given by Eq. (45).
- Fig. 5. Visualization of the characteristic function $g(k)$ (given by Eq. (33)), which determines the kernel of the Gelfand-Levitan integral equation. As can be seen, $g(k) = 1$ (with very high precision) if $k \lesssim k_0 = \sqrt{V(0)/C}$ (see Fig. 4 to understand the reason for this), then starts to decrease, gradually "breaking free" from the potential field, and $g(k) \rightarrow 0$ as $k \rightarrow \infty$. In spite of the seeming simplicity of the energy dependence, the whole curve has to be (and has been) calculated very accurately up to very high energies, in order to accurately ascertain the potential. The high-energy part of the curve ($k \geq k_a$) has been calculated according to Eq. (44).

TABLE 1. Parameters of the three-component reference potential for Xe_2 (first column) and its discrete energy eigenvalues E_n .

Units used:	n	E_n (meV)
V_k ($k = 0, 1, 2$) - meV	0	-23.043278
D_k - meV	1	-20.618294
α_k - $1/\text{\AA}$	2	-18.347033
r_k, X_1, X_2 - \AA	3	-16.229494
	4	-14.266840
$V_0 = -38.865765625809$	5	-12.457771
$D_0 = 0.02078293632204$	6	-10.802778
$R_0 = 6.23549082364147$	7	-9.301735
$\alpha_0 = 1.61583465987087$	8	-7.954433
	9	-6.760559
$V_1 = -24.3134155$	10	-5.718592
$D_1 = 21.629$	11	-4.817731
$R_1 = 1.5537$	12	-4.028060
$\alpha_1 = 4.3634$	13	-3.328990
	14	-2.712825
$V_2 = 0.0155845$	15	-2.171217
$D_2 = -V_2$	16	-1.698210
$R_2 = 0.3755186$	17	-1.289229
$\alpha_2 = 14.05149$	18	-0.940193
	19	-0.647734
$X_1 = 4.00000$	20	-0.409167
$X_2 = 6.05149$	21	-0.222466
	22	-0.086525
	23	-0.002574

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